

## REMARKS/ARGUMENTS

### *Claim Rejections - 35 USC § 101*

The Examiner has not found Applicants' arguments submitted in response to the last and prior Office Actions persuasive and has maintained the 35 U.S.C. § 101 rejection with respect to claims 1 – 3 and claims 10 – 12.

Applicants continue to believe that the claims do define patentable subject matter and in support of that belief present the following comments.

#### Examiner's Rejection:

The Examiner notes that the applicants amended the claims to move a phrase from the preamble to the end of the claim as a “wherein” clause. Additionally, the Examiner notes that:

“...This phrase is not sufficient to produce a concrete, tangible useful result, and does not render the product itself, the virtual library, statutory subject matter. This describes the virtual library, and proposes an intended use for the library. Statements of intended use do not materially affect the nature of the product.”

Further on the Examiner notes that:

“...Descriptive material can be characterized as either “functional descriptive material” or “nonfunctional descriptive material.” In this context, “functional descriptive material” consists of **data structures and computer programs which impart functionality when employed as a computer component.** (The definition of “data structure” is “a physical or logical relationship among data elements, designed to support specific data manipulation functions.” ... “nonfunctional descriptive material” includes but is not limited to music, literary works and a compilation or mere arrangement of data.” The virtual library of the claims does not perform any function, but is merely a storage of informations. The MPEP further notes: “Where certain types of descriptive material, such as music, literature, art, photographs and mere arrangements or compilations of facts or data, **are merely stored so as to be read or outputted by a computer without creating any functional interrelationship, either as part of the stored data or as part of computing processes performed**

**by the computer**, then such such descriptive material alone does not impart functionality either to the data as so structured, or to the "computer." (Emphasis added).

Applicants' Response:

Applicants understand the Examiner's comments and appreciate the effort the Examiner has taken to clarify her reasoning. In the amendments to the claims in the prior office action, Applicants moved a phrase from the preamble to the end of the claim as a "wherein" clause to emphasize the functional structure of the virtual library. As stated in the last response:

Applicants believe that both in their prior Response and in the previous additional remarks, they have demonstrated that the structure of the virtual library provides for types of molecular characterizations and searches which heretofore could not be achieved and that this is only possible because the makeup of the virtual library constitutes just such **functional interrelationships** "as part of the stored data or as part of the computing processes performed" as are required to make the invention statutory.

In order to emphasize the fact that it is the functional structure of the virtual library and the manner in which its components are defined that enables the searching, Applicants have amended claims 1, 2, 3, 10, 11, and 12 by removing from the preamble the reference to searching the virtual library for product molecules and placing the recitation at the end of the claim in a "wherein" clause. Amended in this manner, Applicants submit that the functional link between the ability to search and the structure of the virtual library and its components will be more apparent.

The Examiner has indicated that this argument was not persuasive. Apparently, Applicants have failed to adequately convey their reasons for believing that the required functionality exists. Applicants respectfully request the Examiner's patience as Applicants try again to describe their viewpoint. Modern biochemistry recognizes the importance of molecular shape as a principal feature of biochemical interactions. The virtual library of this invention was designed to permit three dimensional shape searching. Starting with a known molecule having

some desired activity, the question can be posed: what other molecules have the same three dimensional shape as the known molecule? From much experience, it is known that molecules of similar shape are likely to possess similar biological activity. To enable shape searching, the virtual library stores a representation of the three dimensional shapes of molecular parts (side chains and central cores) as well as a knowledge of the combinatorial reactions in which the molecular parts may participate. It should also be noted that the position of the open valence or attachment bond of each molecular part is retained so that a shape analysis of possible combinatorially assembled product molecules will be chemically meaningful. These shape representations are biologically meaningful since they are generated by using molecular descriptors validated as possessing a neighborhood property. If all the computer search program did was to read or output the stored data “without creating any functional interrelationship”, then the Examiner *might* be correct that no functionality was imparted.

However, during the search process, the three dimensional shapes of product molecules obtained through a combination of the individual descriptor values can be compared to the shape of the query molecule without the necessity of generating the product structures. The specification teaches how the data in the virtual library is used to achieve this end. Clearly there is “**....a physical or logical relationship among the data elements, designed to support specific data manipulation functions” “which impart functionality when employed as a computer component.”** Applicants respectfully request that the Examiner review Applicant’s prior responses and arguments in view of the above characterization of the virtual library.

In view of the arguments presented, Applicants respectfully request that the 101 rejections be removed.

This ability to estimate and compare the shape of product molecules to a query molecule involves significantly different data elements and their functional interrelationships than are found in Agrafiotis or Horlbeck. Once it is appreciated that the virtual library does not consist of non-functional descriptive material, the differences between the virtual library of this invention and the invention of Agrafiotis are clear. Due to the different process by which the virtual library of the present invention is formed, it can not be anticipated by an entirely different method as taught by Agrafiotis.

Accordingly, Applicants respectfully request that the rejections of claims 1-3 and 10-13 under 35 U.S.C. § 102(e) be removed.

*Claim Rejections - 35 USC § 102(e)*

Examiner's Rejection:

The Examiner has further rejected claim 13 under 35 USC § 102(e) as being anticipated by Horlbeck (USP 5,880,972). The Examiner quotes Horlbeck as teaching a:

“...small molecule combinatorial library planning tool for automatically and intelligently selecting synthons without performing a chemical synthesis...”

Applicants' Response:

Applicants agree that Horlbeck teaches a small molecule combinatorial library planning

Serial No. 09/866,543  
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tool. Horlbeck teaches nothing at all about: 1) characterizing molecular parts with a descriptor validated as possessing a neighborhood property; or 2) constructing a virtual library in which shapes of molecules can be searched; or 3) shape searching a virtual library for molecules having a shape similar to a known query molecule. A word search of the Horlbeck patent finds no reference to either "shape" or "three dimensional" or 3-D. (3D turns up as a figure reference only.) Since none of the attributes of Applicants' invention are taught by Horlbeck, Horlbeck can not anticipate Applicants' invention.

Accordingly, Applicants respectfully request that the rejections of claim 13 under 35 U.S.C. § 102(e) be removed.

Applicants submit that they have adequately addressed all grounds for rejection raised by the Examiner and respectfully request that a timely Notice of Allowance be issued in this case.

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Respectfully submitted,



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